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UBPKM <-
function(model,fixed.params,which.quantile=0.95,CV.params=NULL,unif.params=NULL,samples=1000)
{
  sample.vec <- rep(NA,samples)
  for (this.sample in 1:samples)
  {
    these.params <- fixed.params
    for (this.param in names(CV.params))
    {
      these.params[[this.param]] <-
rnorm(1,mean=CV.params[[this.param]]$mean,sd=CV.params[[this.param]]$mean*CV.params[[this.param]]$CV)
    }
    for (this.param in names(unif.params))
    {
      these.params[[this.param]] <-
runif(1,min=unif.params[[this.param]]$min,max=unif.params[[this.param]]$max)
    }
    sample.vec[this.sample] <- call(model,these.params)
  }

  return(quantile(sample.vec,which.quantile))
}

Calc_1comp_Css <- function(chem.name=NULL,chem.CAS=NULL,daily.dose=1,which.quantile=0.95)
{
}

Wetmore_Css <-
function(chem.name=NULL,chem.CAS=NULL,daily.dose=1,which.quantile=0.95,species="Human",clearance.assay.conc=1,units="mgperL")
{
  if (!(which.quantile %in% c(0.05,0.5,0.95))) stop("Wetmore papers only includes 5%, 50%, and 95% quantiles.")
  if (!(units %in% c("mgperL","uM"))) stop("Wetmore papers only includes mgperL and uM values for Css")
  if (is.null(chem.CAS) & is.null(chem.name))
  {
    stop("Must specify compound name or CAS.\n")
  } else if ((!is.null(chem.CAS) & !any(Wetmore.data[,"CASRN"]==chem.CAS)) & (!is.null(chem.name) & !any(Wetmore.data[,"Compound"]==chem.name)))
  {
    stop("Compound not found.\n")
  } else {
    if (!is.null(chem.CAS)) chem.name <-
Wetmore.data[Wetmore.data[,"CASRN"]==chem.CAS,"Compound"][1]
    else chem.CAS <- Wetmore.data[Wetmore.data[,"Compound"]==chem.name,"CASRN"][1]
    this.data <-
subset(Wetmore.data,Wetmore.data[,"CASRN"]==chem.CAS&Wetmore.data[,"Concentration..uM."]==clearance.assay.conc&Wetmore.data[,"Species"]==species)
    if (dim(this.data)[1]!=1) stop(paste("No",clearance.assay.conc,"uM clearance assay data for",chem.name,"in",species))
    if (units=="mgperL")
    {
      if (which.quantile==0.05) return(daily.dose*this.data[,"Css_lower_5th_perc.mg.L"])
      else if (which.quantile==0.5) return(daily.dose*this.data[,"Css_median_perc.mg.L"])
      else return(daily.dose*this.data[,"Css_upper_95th_perc.mg.L"])
    }
  }
}

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} else {
  if (which.quantile==0.05) return(daily.dose*this.data[,"Css_lower_5th_perc.uM."])
  else if (which.quantile==0.5) return(daily.dose*this.data[,"Css_median_perc.uM."])
  else return(daily.dose*this.data[,"Css_upper_95th_perc.uM."])
}
}
}

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Wetmore_Css(chem.CAS="94-82-6")
Wetmore_Css(chem.CAS="94-82-6",which.quantile=0.95)

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Wetmore_Oral_Equiv <-
function(conc,chem.name=NULL,chem.CAS=NULL,suppress.text.output=F,which.quantile=0.95,species=
"Human")
{
  if (conc < 5) this.conc <- 1
  else this.conc <- 10
  Css <-
try(Wetmore_Css(chem.name=chem.name,chem.CAS=chem.CAS,which.quantile=which.quantile,species
=species,clearance.assay.conc=this.conc))
  if (class(Css) == "try-error") return(NA)
  else {
    return(conc/Css)
  }
}

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Wetmore_Oral_Equiv(4,chem.CAS="94-82-6")
Wetmore_Oral_Equiv(6,chem.CAS="94-82-6")
Wetmore_Oral_Equiv(6,chem.CAS="94-82-6",species="Rat")

```